Quantum Dot Modeling using NEMO 3-D

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Work performed in collaboration with
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Tim Boykin (U Alabama in Huntsville)

Presentation Outline

- NASA Mission Pull
- Technology Push:
- What is a Quantum Dot ?
- Our Project portfolio
  - Modeling / Characterization / Applications
- Quantum Dot Modeling:
  - Tight Binding Parameterization
  - Strain
  - Alloy Disorder
  - Interface Interdiffusion
- NEMO 3-D:
  - Parallelization, Nanotubes, GUI

2004-2015 Mission Pull

Solar System Exploration near-term

- Pluto (04)
- Europa orbiter (06)
- Solar Probe (07)

Solar System Exploration long-term

- Comet nucleus sample return
- Europa lander
- Titan explorer

Structure and Evolution of the Universe (SEU)

- 14 projects

Sun Earth Connection (SEC)

- 10 projects

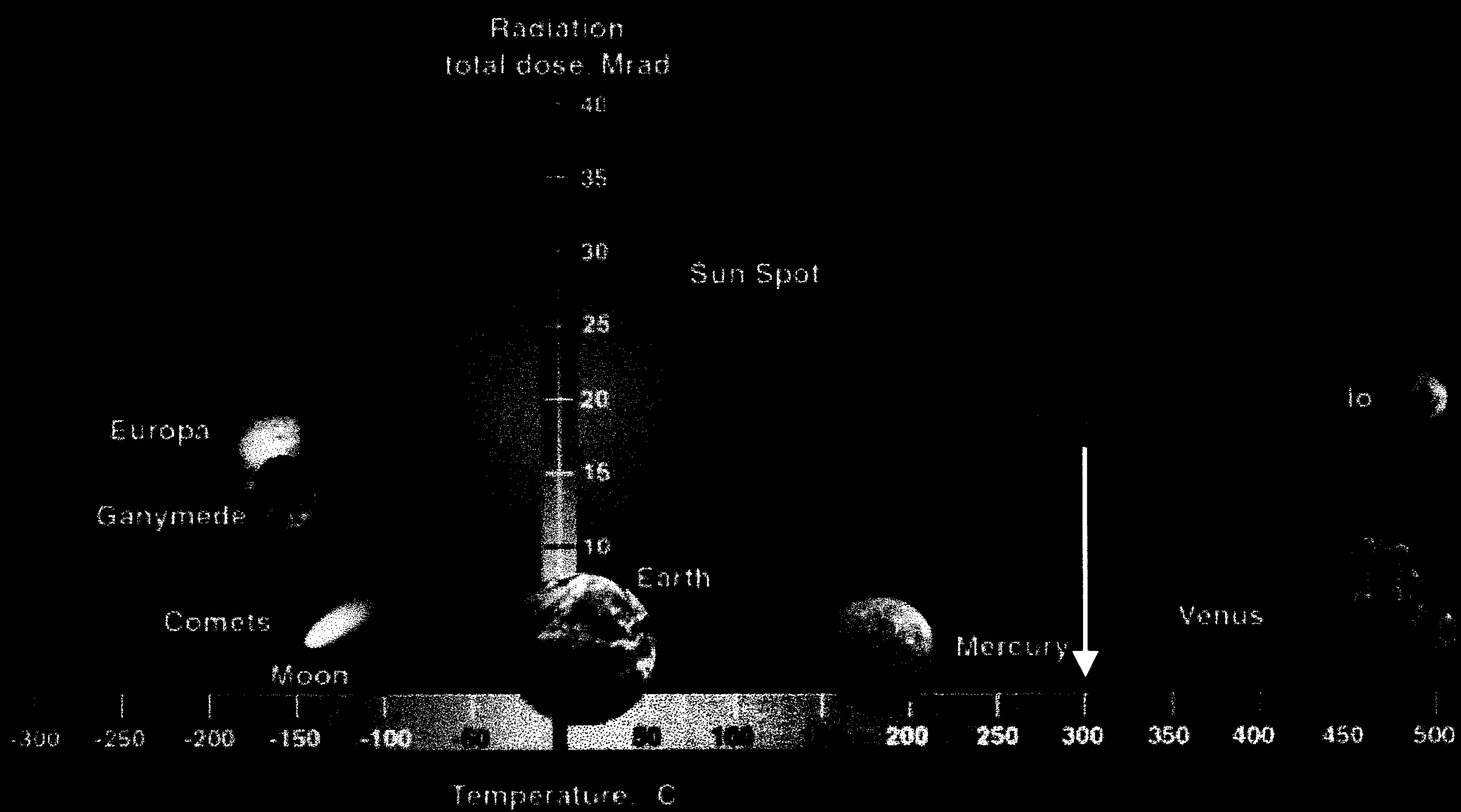
General Technology Requirements

- High radiation tolerance
- Extreme temperature operation
- Low weight, low power, high performance, high capacity

Defined IT Requirements

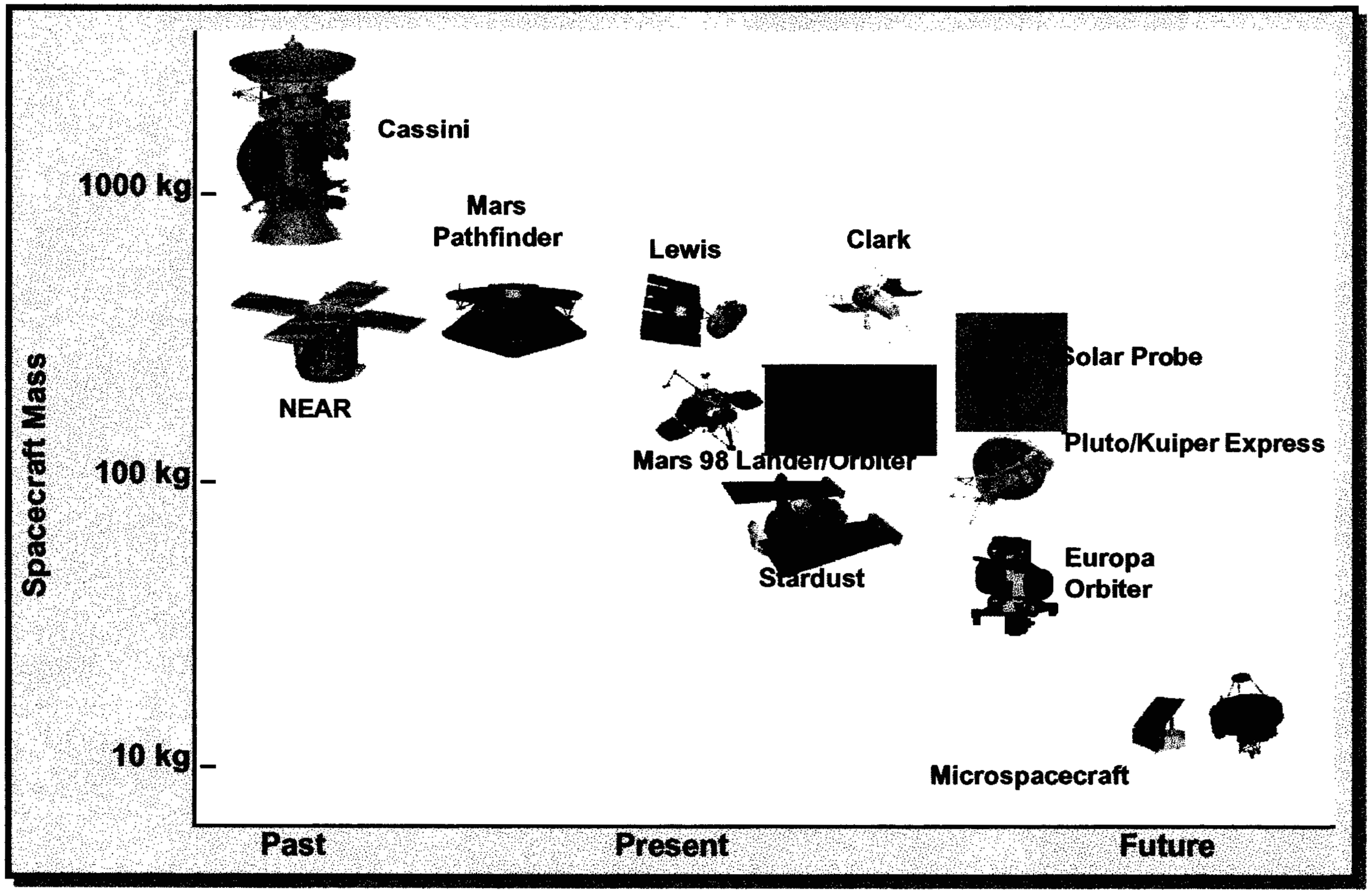
- Closed loop autonomous Guidance Navigation and Control
- Formation flying
- Data Fusion
- Data Timing Synchronization
- Science feature detection
- Science alert capability
- Data synthesis and visualization

Planetary Extreme Environments



Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Progressive Spacecraft Miniaturization



Low weight, low power and high efficiency
Have a special meaning to NASA

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Technology Push
Toward Fundamental Limitations

Commercial market pushes computing performance (FLOPS/weight/power):

- Enabled by device miniaturization
- Enabled by chip size increase
- Limited by: Costs of fabrication
- Limited by: Discrete atoms/electrons

Additional NASA Requirements:

- High radiation tolerance
- Extreme temperature operation-hot/cold

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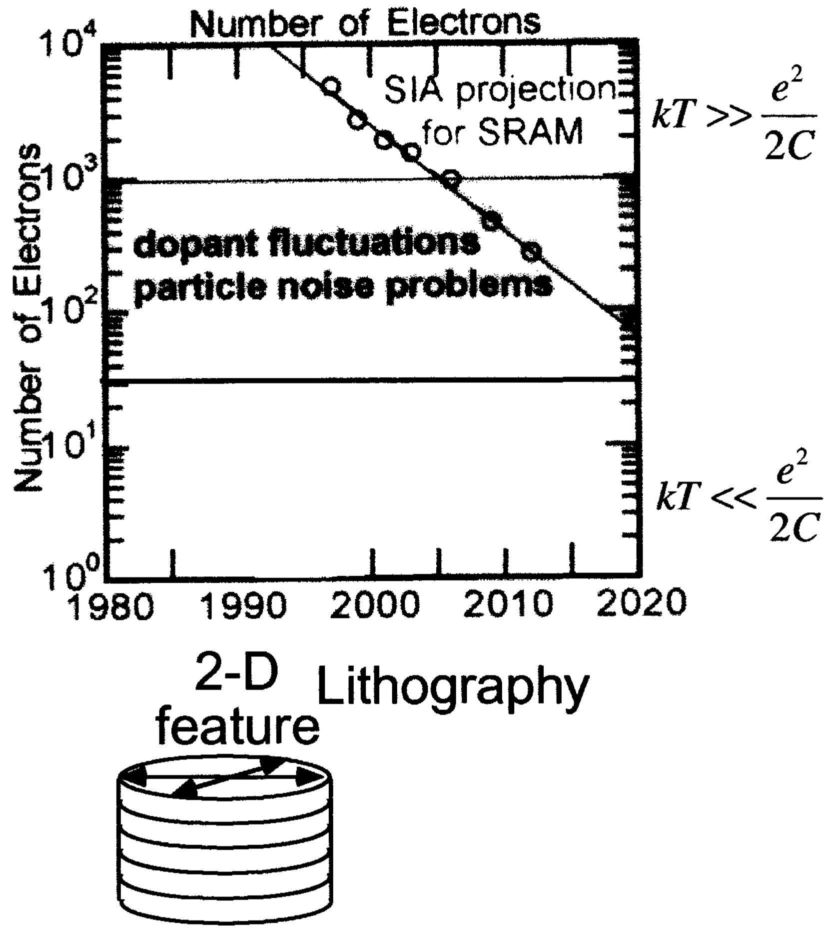

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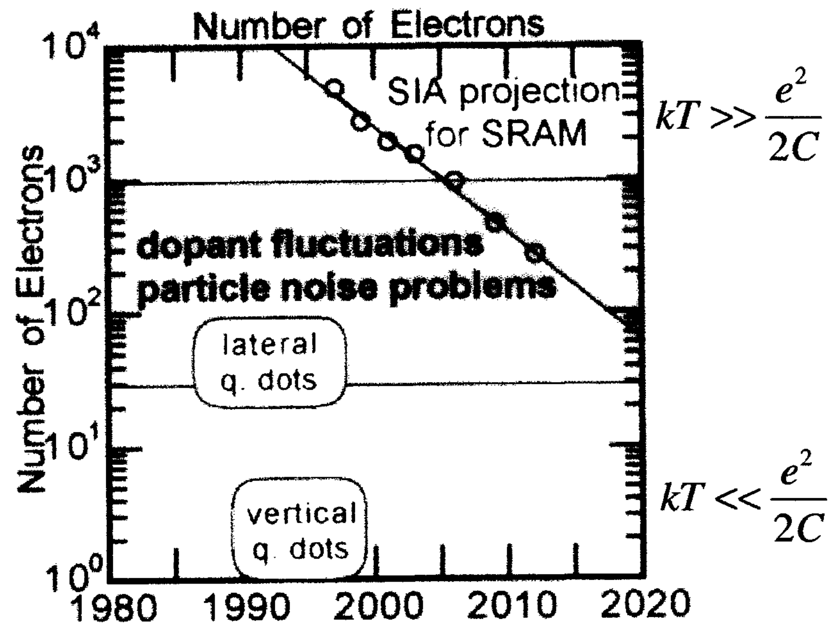

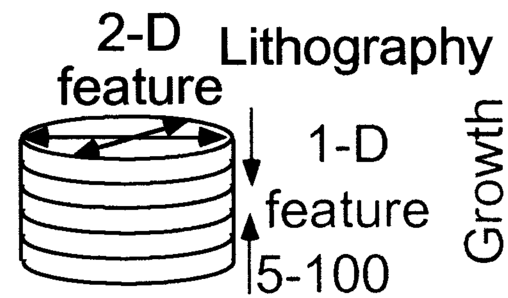

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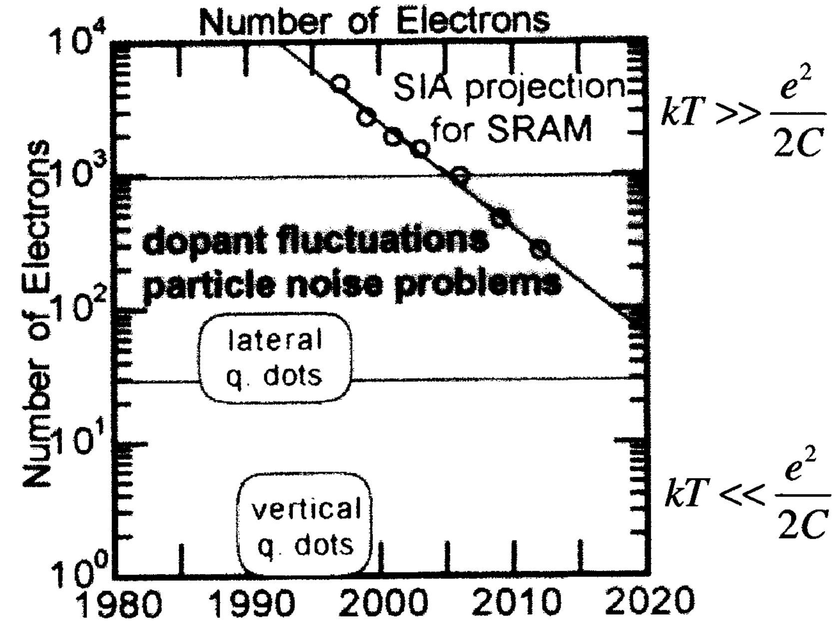
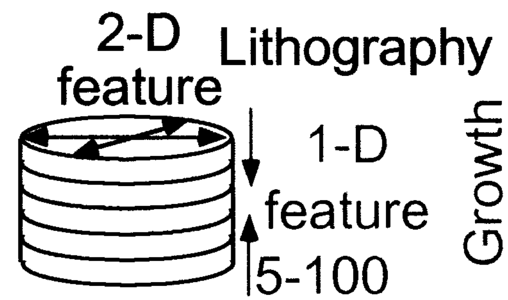
Quantum Dots Push beyond SIA with near and long term applications

- Detectors / lasers
- Memory and logic





Quantum dots go beyond the SIA roadmap and enable near and long term NASA applications

What is a Quantum Dot ?
Basic Application Mechanisms

Physical Structure:

- Well conducting domain surrounded in all 3 dim. by low conducting region(s)
- Domain size on the nanometer scale

Electronic structure:

- Contains a countable number of electrons
- Electron energy may be quantized -> artificial atoms (coupled QD->molecule)

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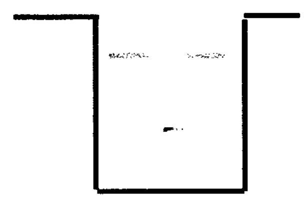

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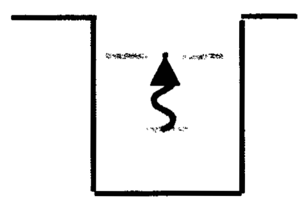

Photon
Absorption

↓

**Detectors/
Input**

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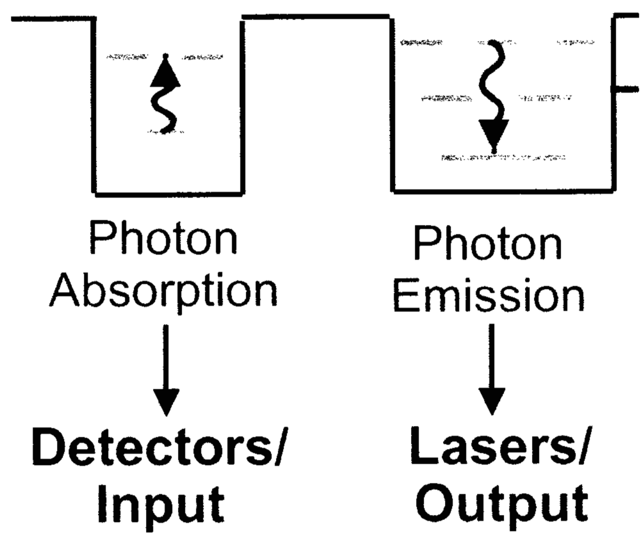

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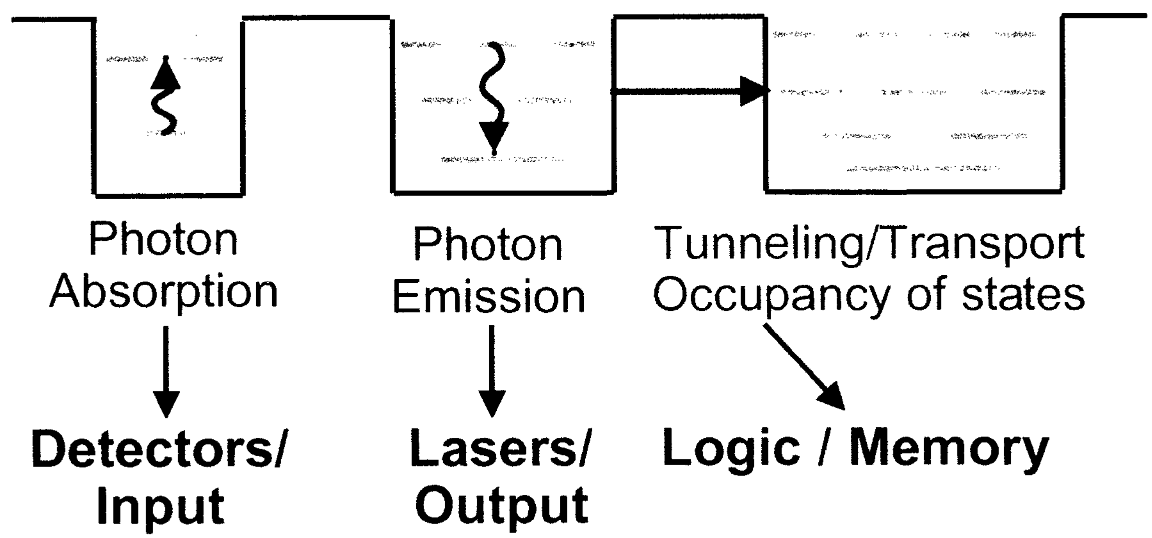

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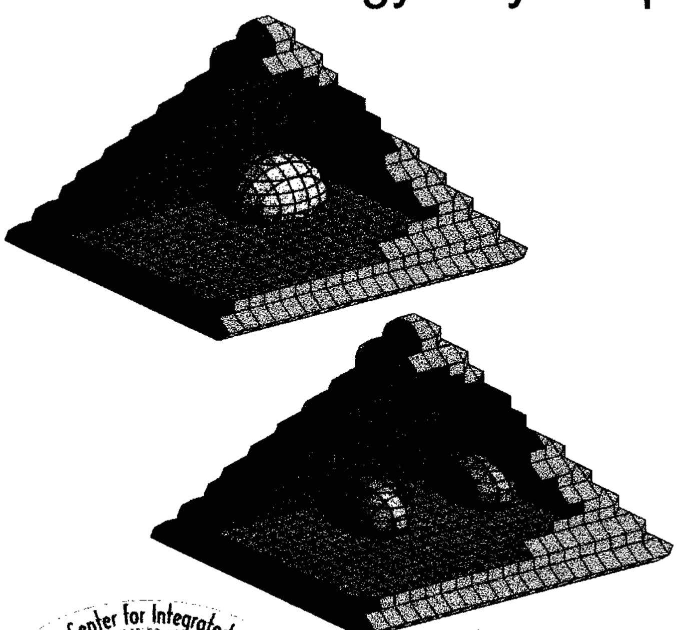

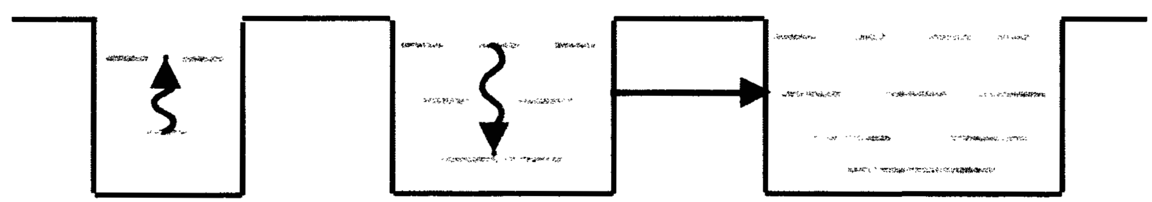

Photon Absorption → **Detectors/ Input**

Photon Emission → **Lasers/ Output**

Tunneling/Transport Occupancy of states → **Logic / Memory**

Quantum dots are artificial atoms that can be custom designed for a variety of applications

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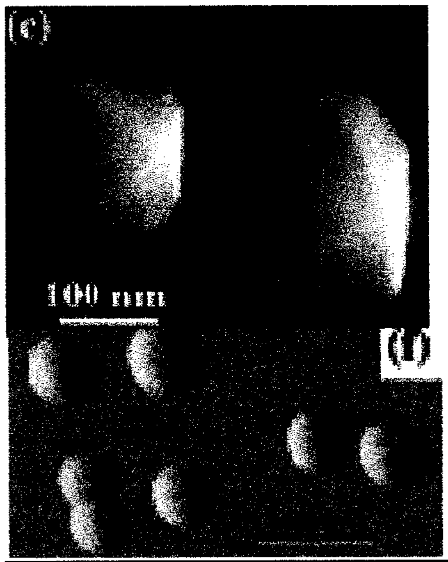
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

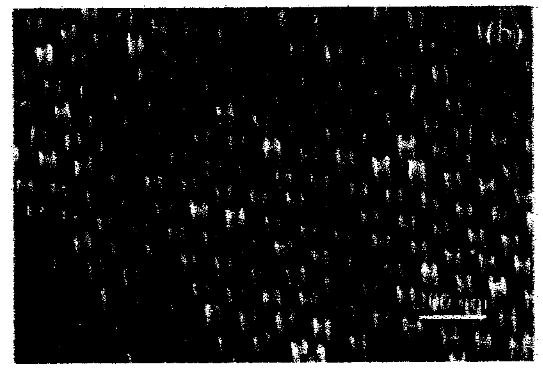
Nanotechnology / Nanoelectronic Example Implementations



Self-assembled , InGaAs on GaAs.

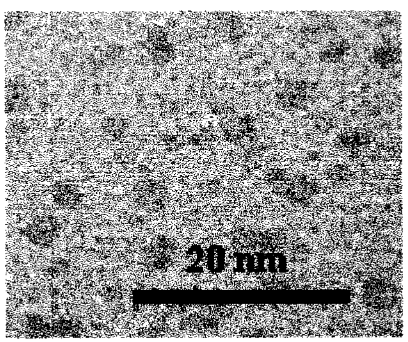
Pyramidal or dome shaped

R.Leon,JPL(1998)



Nanotube Arrays,

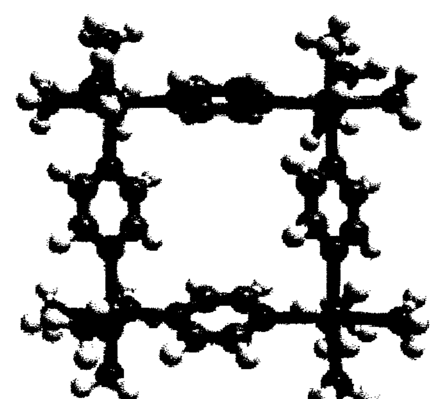
Jimmy Xu, Brown Univ. (1999)



Nanocrystals:

Si implanted in SiO_2

Atwater, Caltech (1996)



Molecular Dots
Ruthenium-based molecule Ru4(NH3)16(C4H4 N2)410+ proposed by Marya Lieberman, Notre Dame (1999)

Low Dimensional quantum confinement can be achieved in a variety of material systems

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Nanotechnology Project Portfolio

- **Modeling**
  - Enable the exploration of the nanotechnology design space.
- **Characterization**
  - Optical, structural, transport and radiation testing.
- **Devices**
  - **Lasers / Output:** Enable radiation hard, narrow linewidth tunable lasers.
  - **Sensors / Input:** Enable acoustic and electronic sensors based on nanotubes.
  - **Memory:** Enable high density, low power, non-volatile, radiation hard storage.
- **Architectures:**
  - Enable massively parallel and fault tolerant computing architectures.

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Future deep space applications will directly benefit from directed nanotechnology research

Need for Quantum Dot Simulation

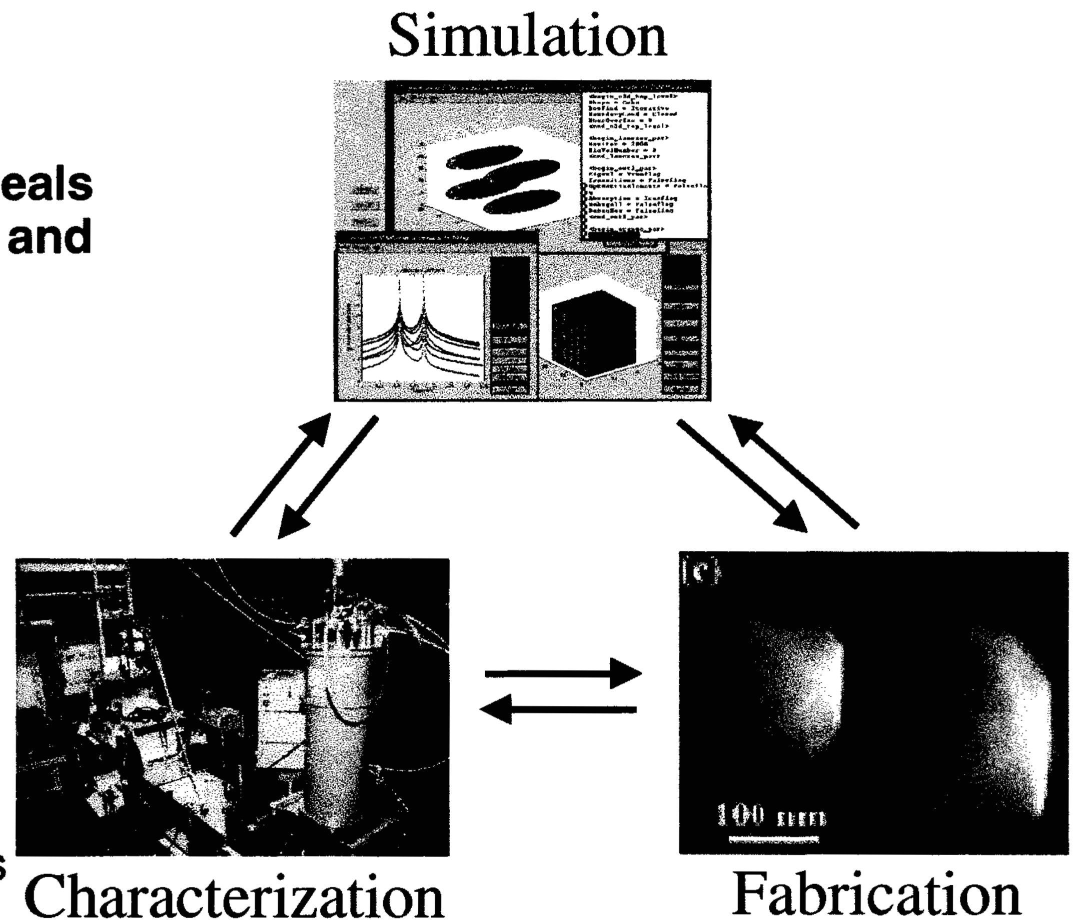
Problems:
- **Design space is huge**
  - **Choice of materials, shapes, orientations, dopings, heat anneals**
- **Characterizations are incomplete and invasive / destructive**

Simulation Impact:
- **Aide Design**
  - **Fast, cost effective.**

  -> Device performance
  already successful for 1-D quantum devices

- **Aide Characterization**
  - **Non-invasive**
  - **More accurate**

  -> Structure and doping analysis
  already successful for 1-D quantum devices



Modeling, Characterization and Fabrication are inseperable for nanoscale devices

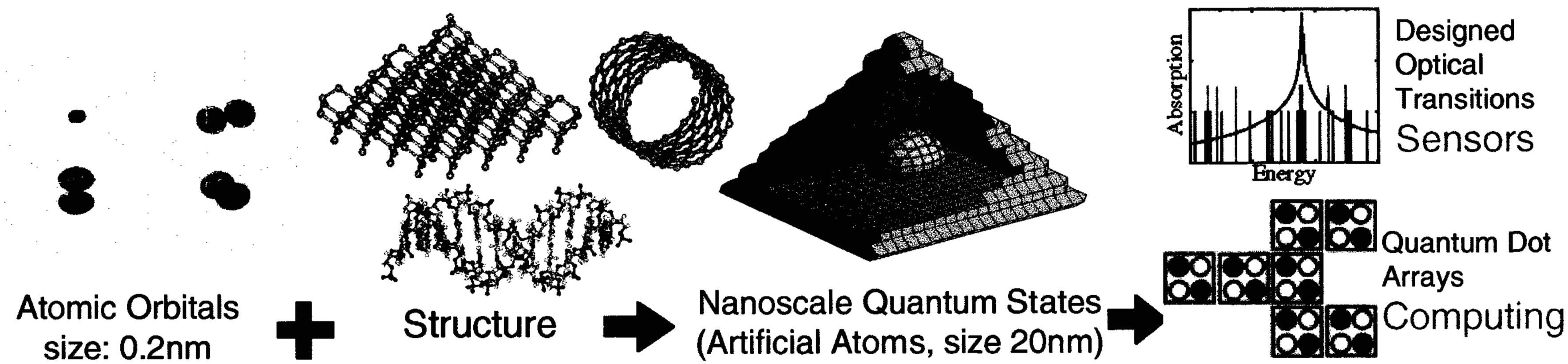
Objective

- **Long term objective:**
  - Develop and demonstrate a physics-based, atomistic simulation tool for semiconductor quantum dots and molecular based electronic devices
- **Near term objective:**
  - Develop this year the technology necessary to simulate optical transitions in a single quantum dot
- **Tasks in FY 00:**
  - Alloyed dot simulation (04/00)
  - Shared memory parallelization (05/00)
  - 3-D visualization (05/00)
  - Atomistic grading simulation (07/00)
  - Atomistic impurity simulation (09/00)

We build a bottom-up, atomistic nanelectronic design tool

Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Quantum Dot Modeling for Revolutionary Computing and Sensing



Opportunity:

- Nanoscale electronic structures can be built!
  => Artificial Atoms / Molecules

Problem:

- The design space is huge: choice of materials, compositions, doping, size, shape.

Approach:

- Deliver a 3-D atomistic simulation tool
- Enable analysis of arbitrary crystal structures, atom compositions and bond/structure.

NASA Relevance:

- Enable devices needed for NASA missions beyond existing industry roadmap:
  - 2-5μm Lasers and detectors
  - High density, low power computation (logic and memory)
  - Life signature biosensors

Impact:

- Low cost development of revolutionary technology.
- Narrow empirical/experimental search space

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Modeling will narrow the empirical search space!

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Related Work

Investigator	Location	Hamiltonian	Atomistic	Many-Body	Extendable to Molecules?
Pryor	Lund	k•p	NO	YES	NO
Bimberg	Berlin	k•p	NO	NO	NO
Freund	Brown	k•p	NO	NO	NO
Leburton	Illinois	1 Band	NO	NO	NO
Zunger	NREL	Pseudopotential	YES	NO	NO
Bowen/Klimeck	JPL	Tight-binding	YES	NO*	YES

* - Planned for 01

Why JPL? JPL has expertise and infrastructure to tackle such large problems.

We are in a excellent position to simulate molecular electronics from the bottom -up

Technical Accomplishments (Physics)

- Genetic algorithm based material parameter analysis
  - Establish a material basis set needed for atomistic simuations
- Mechanical strain calculation
  - Enable proper modeling of optical bandgaps
    -> proper tuning of optical transitions
- Alloyed Dot simulation
  - Enable simulation of realistic quantum dot compositions
  - Enable analysis of inhomogeneous linewidth broadening due to alloy disorder
- Atomistic grading simulation
  - Enable simulation of realistic quantum dot interfaces
  - Enable simulation of interface interdiffusion and the resulting modification of the confined quantum states.

We are just starting to explore the capabilities of this simulator!

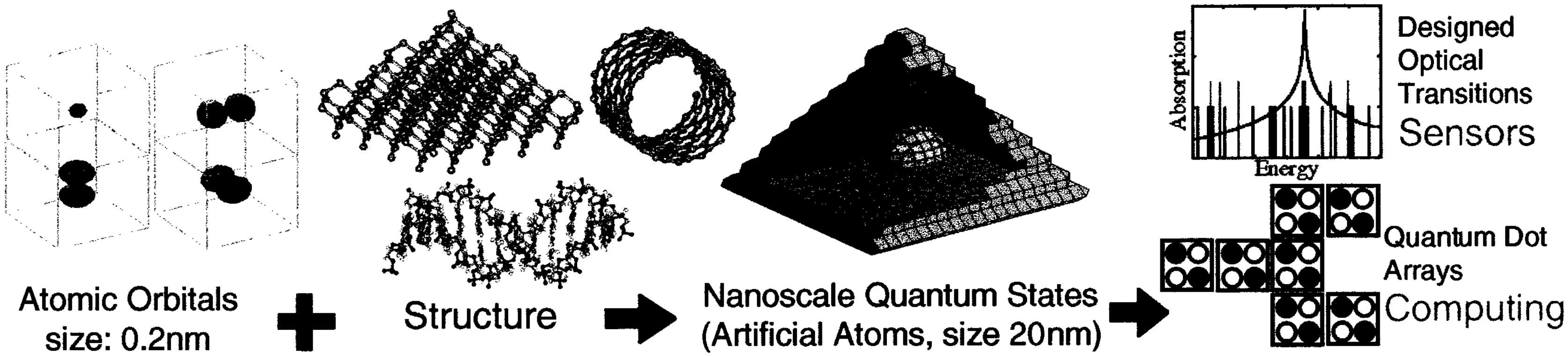
Technical Accomplishments (Software)

- Parallelization
  - Evaluate performance of 2 different parallel computing paradigms:
    - shared memory (all CPUs can access the same memory)
    - distributed memory (message passing between CPUs)

  => performed a 2 million atom simulation in the distributed model
- Analysis of general molecular inputs -> Nanotubes
  - Enable electronic simulation of "arbitrary" crystal structures generated from other structural simulators.
    -> Expansion to Moletronics
- Graphical User Interface Prototype
  - Enable device, material and computer specific input to and output from a supercomputer based simulator.
- 3D Data Visualization
  - Enable visualization of simulation results

3 person years of software work at JPL and 22 person years NEMO leverage enabled the simulation capabilities.

Technical Approach



Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extend, not infinitely periodic
  => local orbital approach
- Need to include about one million atoms.
  => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape.
  => need a design tool

Approach:

- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals depending on the material.
  - Use genetic algorithm to determine material parameter fitting
- Compute mechanical strain in the system.
- Develop efficient parallel algorithms to generate eigenvalues/vectors of very large matrices (N=40million for a 2 million atom system).
- Develop prototype for a graphical user interface based nanoelectronic modeling tool (NEMO-3D)

Realistic material description at the atomic level enables simulation of realistic nanoelectronic devices.

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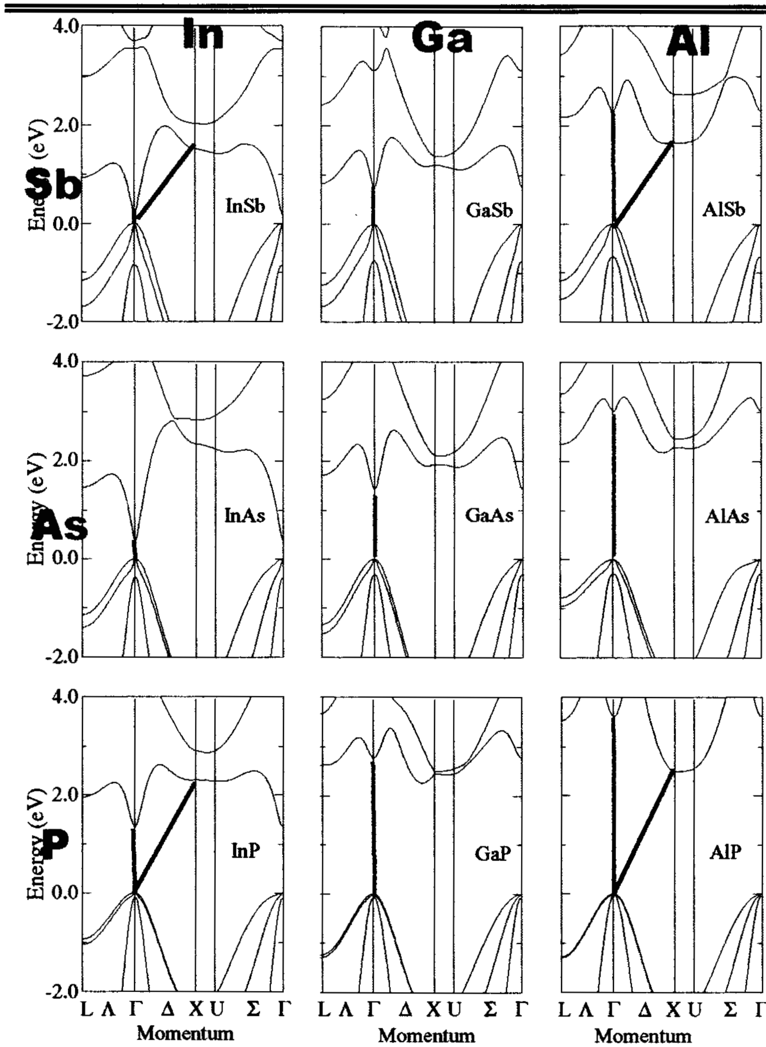
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Genetic algorithm based material parameter analysis



Problem:

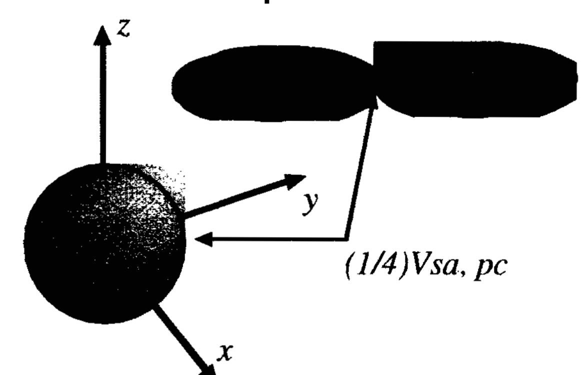
- Want atomistic / orbital based material description.
- Need to fit 15-30 orbital interaction energies to 20-30 material properties (bandgaps and masses)

Approach:

- Use massively parallel genetic algorithm to perform multidimensional optimization

Results/Impact:

- Established a 3x3 array of materials and their parameters that are the building blocks of quantum dots.
- Enable the atomistic simulation of quantum dots.



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Genetic algorithm enabled the establishment of a material basis set.

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Mechanical Strain Calculations

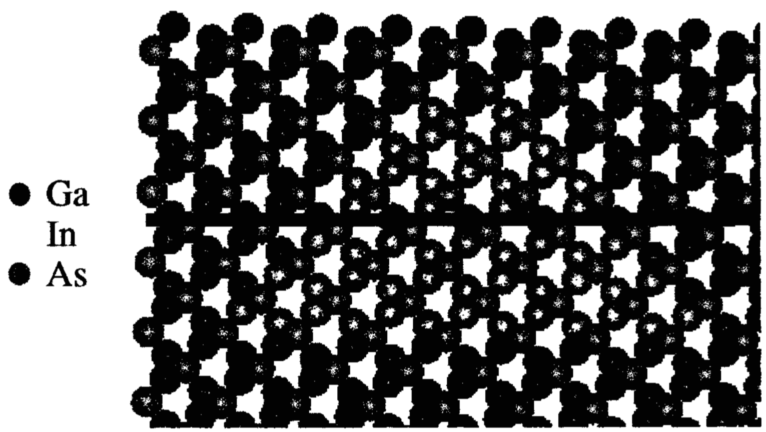
Problem:
- Self-assembly dot formation due to strain
- Small mechanical strain (5% bond length) -> dramatic effects on electronic structures

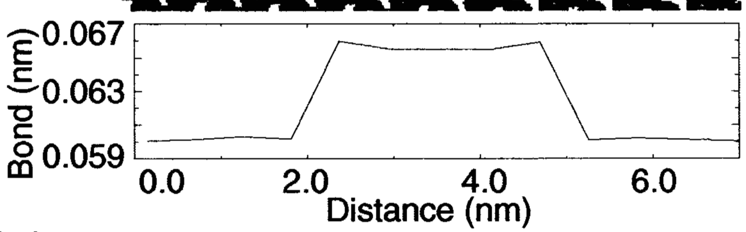
Approach:
- Nanomechanical strain calculation
- Nanoelectronic strain calculation.

Results:
- Implemented a mechanical strain model.
- Implemented atomistic bandstructure model that comprehends strain.

Impact:
- Can simulate realistic quantum dots.
- Can estimate optical transition energies properly.

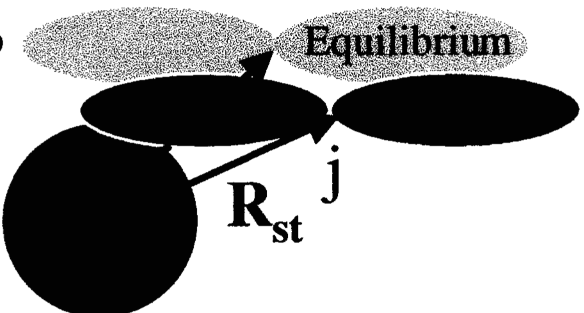
Mechanics Problem: Minimize elastic strain (Keating)

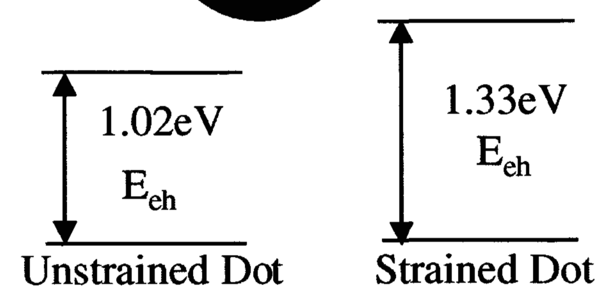




Electronics Problem: Effect of overlap changes

Orbital overlap changes => bandgaps and masses





Pyramidal InAs Dot Simulation

Base: 7nmx7nm Height: 3nm Embedded in GaAs

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Small strain has dramatic effects on the electronic structure.

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Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

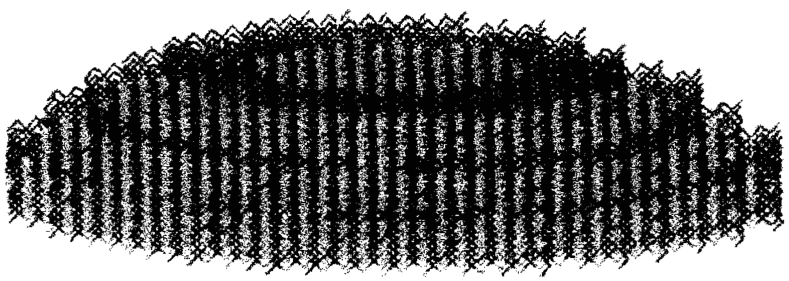
Alloy Disorder in Quantum Dots

Problem:
- Cations are randomly distributed in alloy dots.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?

Approach:
- Simulate a statistical ensemble of alloyed dots.
- Requires atomistic simulation tool.

Results:
- Simulated 50 dots with random cation distributions.
- Inhomogenious broadening factor of 9.4meV due to alloy disorder.

Impact:
- Fundamental uniformity limit for ensemble of alloy-based quantum dots.

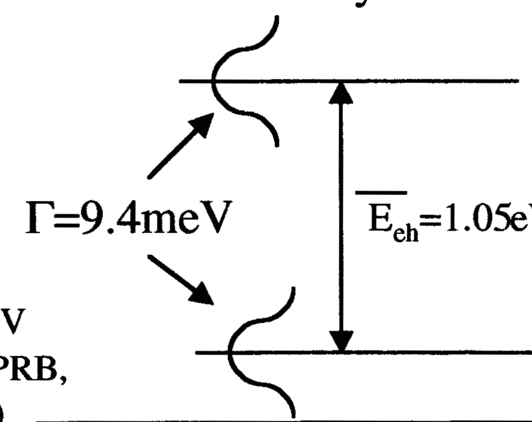


$In_{0.6}Ga_{0.4}As$ Lense Shaped Dot

(Diameter=30nm, Height=5nm, GaAs embedded)

In and Ga atoms are randomly distributed
Inhomogenious Broadening?

Simulation of Alloy Dot Ensemble



Measured
Γ=34.6 meV
(R. Leon, PRB, **58**, R4262)

9.4meV Theoretical Lower Limit

Alloy disorder presents a theoretical lower limit on optical linewidths

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Atomistic Grading Simulation

Problem:
- Quantum dot interfaces may not be sharp.
- There may be cation redistribution around the interface => grading of the concentration.
- How does the interfacial grading affect the electronic structure?

Approach:
- Simulate quantum dot atomistically with graded interfaces as a function of interdiffusion length.

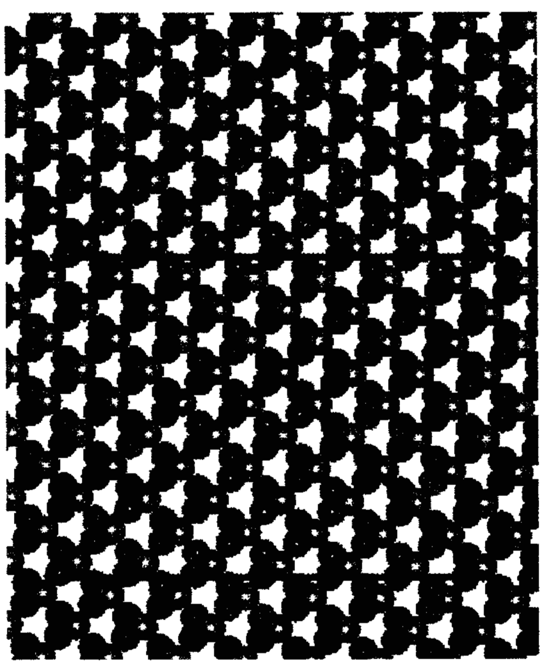
Results:
- More Ga in the quantum dot raises the energy of the transition energies.
- Less Ga in the barriers softens the barriers, reduces the binding of the excited states to the quantum dot and reduces $\Delta E=E_2-E_1$.

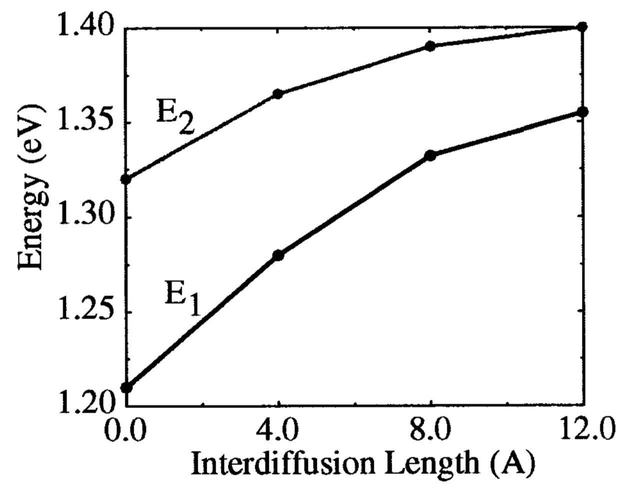
Impact:
- Verify experimentally suggested interdiffusion process may be responsible for blue shift and reduction in ΔE.

Cartoon Visualization of Interdiffusion

Slice through 2 Qdots with thickness of 3 atoms - with and without interdiffusion

● Ga
In
● As





Pyramidal InAs in GaAs, Diameter=10nm, Height=4.2nm 5 samples per data point

Interdiffusion widens the bandgap => blueshift

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Code Parallelization

Problem:

- Need to calculate eigenvalues of a complex matrix of the order of 40 million.
  => must parallelize code

Approach:

- Evaluate 2 parallel programming paradigms
  - Shared memory (OpenMP) - CPUs can access the same memory.
  - Distributed memory - CPUs exchange data through messages (MPI) - data synchronization performed explicitly by program.

Vision:

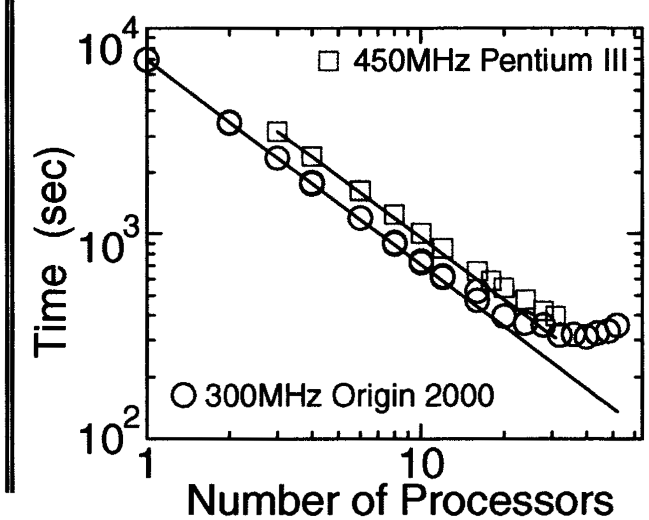
- Utilize a designated beowulf cluster of PC's as a workhorse for these simulations. Each node might have 1-4 shared memory CPUs on one motherboard.
- Envision a "mixed" code with outer level MPI parallelism and inner level OpenMP parallelism.
  - This will run on a commercial supercomputer like an SGI Origin 2000 as well as a beowulf.

Results:

- Inner level OpenMP parallelism does not speed up code significantly. Dynamic creation and destruction of threads is too expensive.
- Decided to abandon the OpenMP implementation and concentrate on the optimization and scaling of the MPI version.

Impact:

- Enabled simulation of 2 million atom systems with 20 orbitals on each atom
  => matrix of order 40million



Compare Origin 2000 vs. Beowulf:

10 Lanczos Iterations for a 1million atom system.

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Cluster of commodity PC's can beat a supercomputer for our problem

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Incorporate Arbitrary Molecular Files ->Nanotubes

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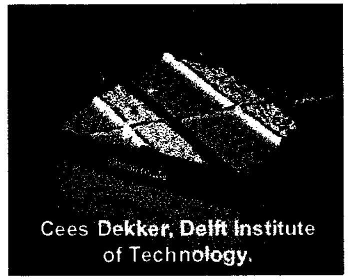
Background:

- Carbon Nanotubes are currently explored for electronic and structural applications.



Objective/Motivation:

- Simulate optical interactions and electron transport in nanotubes

Problem:

- Need nanotube structural information.
- We do not have that expertise.

Approach:

- Expanded code to read standard chemical structure file format.
- Get structural information from other researchers.

Result:

- Simulated nanotube ground states and density of states.

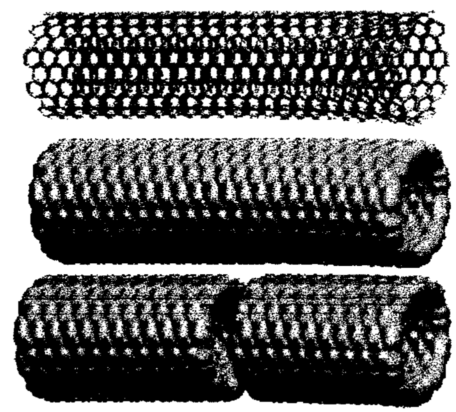
Possible Cooperation from Nanospace 2000 Conference:

Optical Characterization Rice	↔	Structural Simulation Ames, Bonn

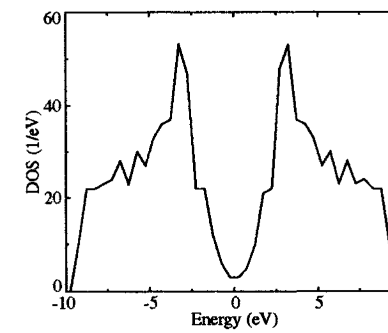
↓ ↓

Electronic/Optical Simulation JPL

Preliminary Data



Finite size nanotube ground and excited state



Density of States

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We can input molecular dynamics based files and perform electronic structure calculations

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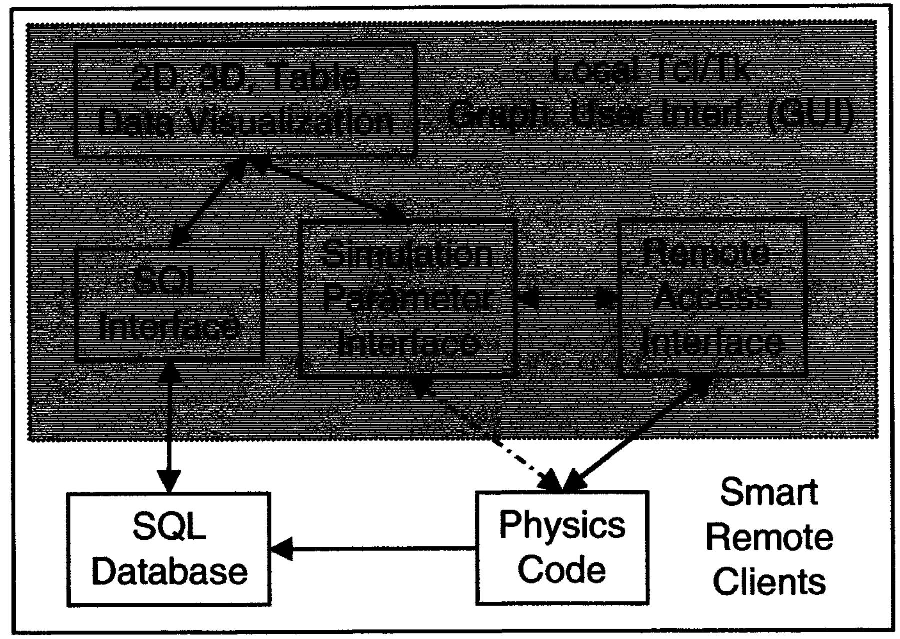
Software Structure Prototype/Vision

Objective:
- Design, develop, test and deliver an interactive quantum dev. design tool
- Customers: Experimentalists not Simulation Specialists !

Problem:
- Simulations are CPU intensive -> need supercomputers
- Datasets are typically 4-dim ->need custom visualization
- Local workstations are PC, MAC, SUN or SGI ->need portable Graph. User Interf.
- Input requirements change fast ->need dynamic GUI design

Approach:
- Heterogeneous client-server Tcl/Tk-based GUI

Impact:
- Using this approach on 2 completely independent simulators with little additional development time.



Smarts are OUTSIDE **the GUI:**
- Physics code contains I/O structures
- Database completely general

-> GUI retrieves I/O structures and data from smart clients.

-> Flexibility for user and developer

Flexible software design enables use in various different simulators

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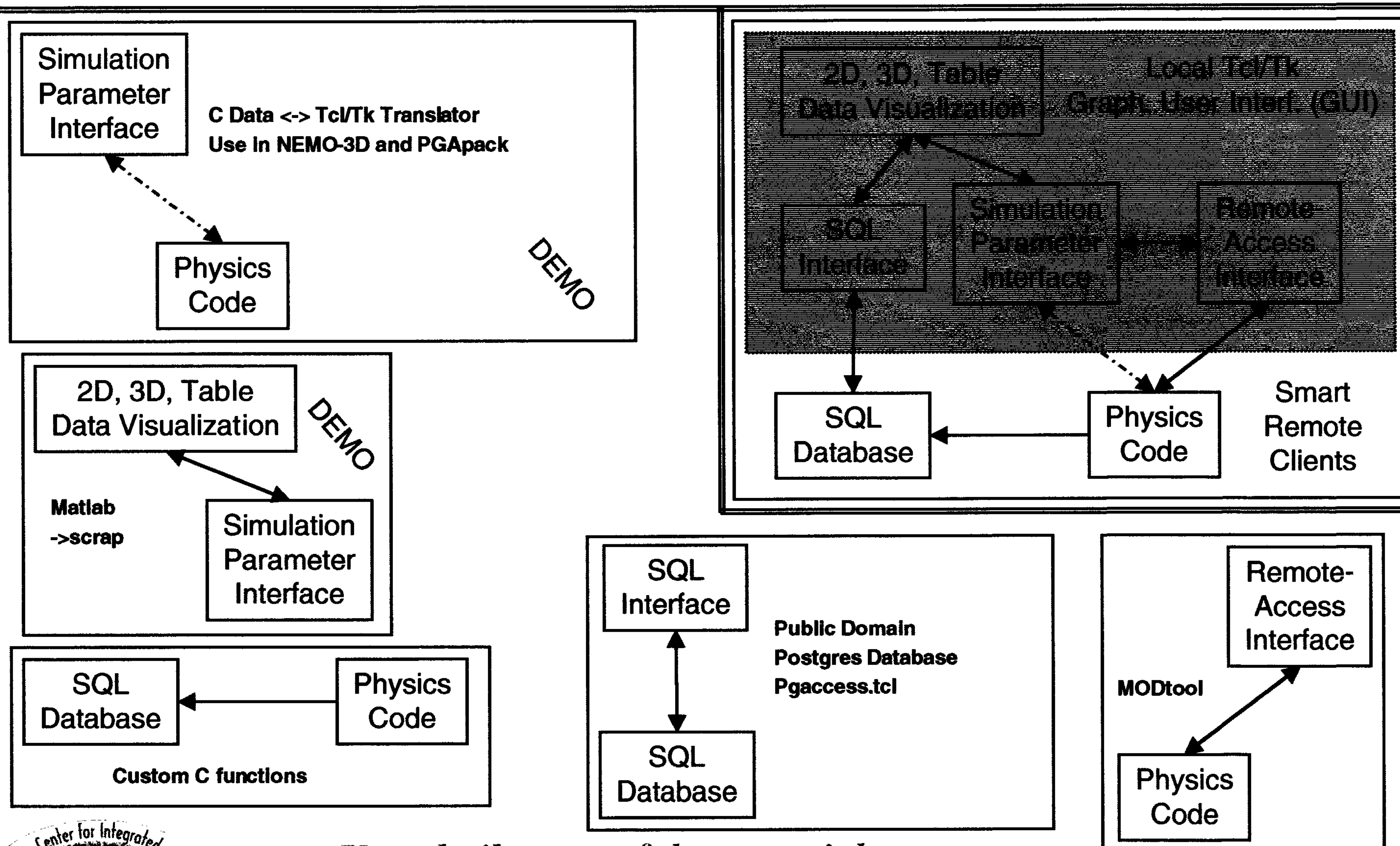
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Software Structure Status



Have built most of the essential components, need to go through integration process.

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Plans

Plans for FY 01:

- Simulation of ensembles of alloyed quantum dots
  - Study fundamental limit of spectral lines due to alloy disorder
- Simulation of many-body effects via configuration interaction
  - Simulate optical transitions including effects of excitons
- Electron transport through quantum dot
  - Explore design possibilities for electronic transport devices

Plans for FY 02:

- Transport through Nanotubes, DNA including bond deformation effects

Plans for outgoing years:

- Develop a world-class 3-d nanoelectronic modeling tool

JPL

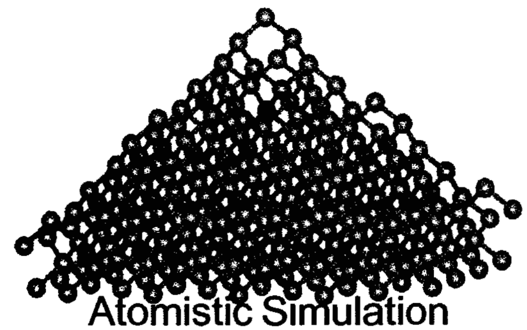
Conclusions / Future Vision

¥Parallelization (2 million atoms), visualization
¥Graded junctions, alloy disorder, strain

¥Made significant progress towards a general atomistic simulation tool

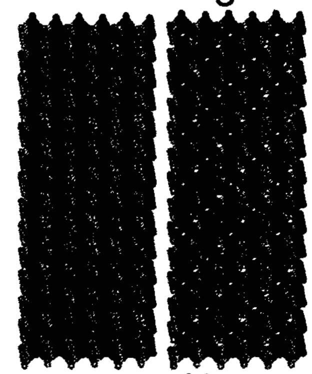
¥Envision this tool to have impact on quantum dots, end of SIA roadmap issues, and molectronics.

Quantum Dots



Atomistic Simulation

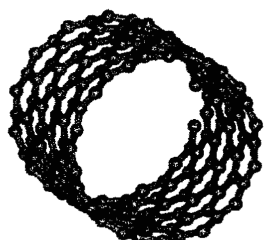
Grading



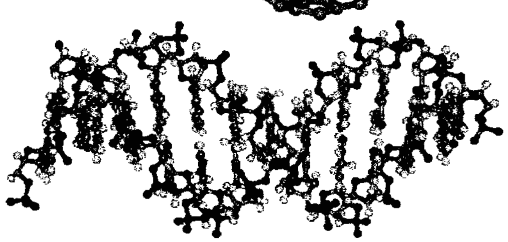
Graded Abrupt

Transport in Molecules

Carbon Nanotubes

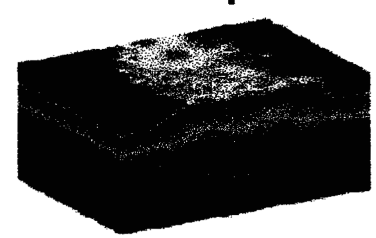


DNA

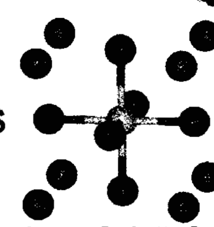


End of SIA Roadmap

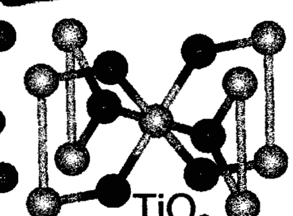
Dopant Fluctuations in Ultra-scaled CMOS



Electron Transport in Exotic Dielectrics



$(Ba,Sr)TiO_3$



TiO_2

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The best is still to come!

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Backup Foils

Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Quantum Dots: Optical and Structural characterization

Task Lead: Rosa Leon

Objectives:

COMPUTERS

- ¥ Quantum Dots can enable new types of computing architectures (for example QCA).

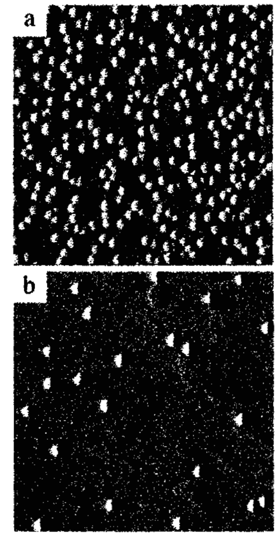
MEMORIES

- ¥ QDs can be used in ultra-high density optical memories.

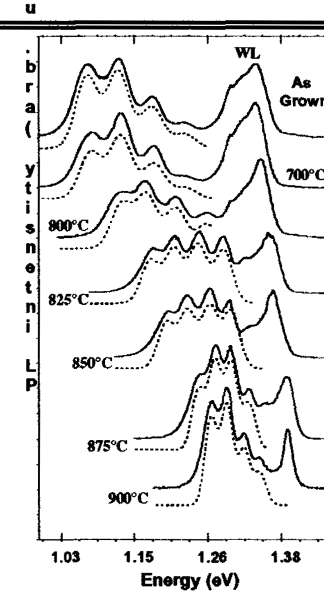
RADIATION TOLERANCE

- ¥ QDs enable radiation-hard opto-electronic devices.

InGaAs Quantum Dots



Squares are 1 µm by 1 µm



Tuning inter-sublevel energies in Quantum Dots

Approach:

- ¥ **Achieve positional order of Quantum Dots (QDs) by combining patterning and various types of growth experiments.**
- ¥ **Implement experimental capabilities for in-house QD characterization.**
- ¥ **Collaborate with Universities on fabrication, growth experiments, and characterization.**
- ¥ **Perform tests and experiments on existing QD structures - understand QD properties and how they impact their various device applications.**

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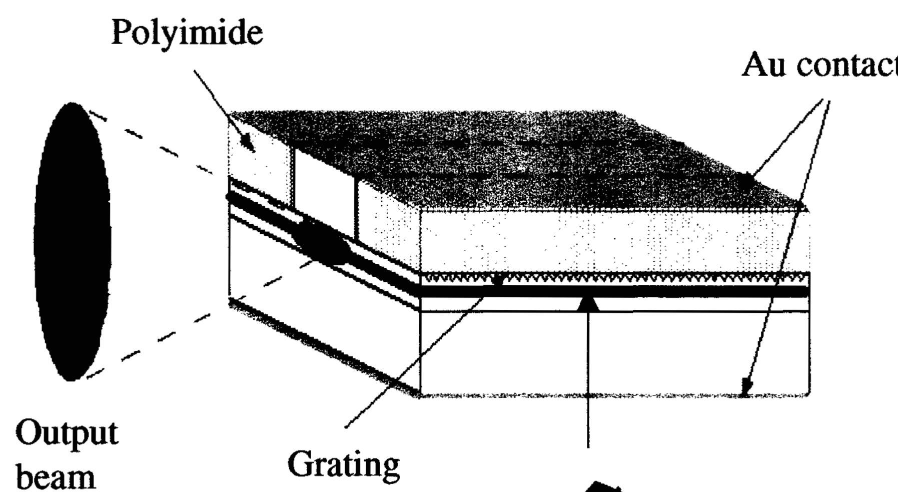
Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Quantum Dot Fabrication for Lasers

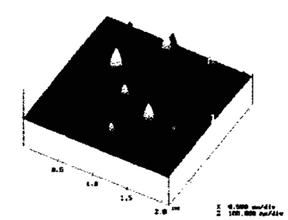
Task Lead: Yueming Qiu

Objective:

- **Design and fabricate high efficient, low power consumption, radiation hard QD based optoelectronic devices, such as:**
  - **lasers**
    - **ultralow threshold current density**
    - **temperature insensitive**
    - **narrow linewidth**



QD active region



NASA applications:

- **Large format, low noise IR detector arrays are enabling technology for SSE**
- **Broad area of applicability:**
  - **Spectroscopy**
  - **Microinstruments**
  - **Communications**
  - **LIDAR and Interferometry**

Collaborators:

- **University of New Mexico**

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Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Single Electron Nonvolatile Memory

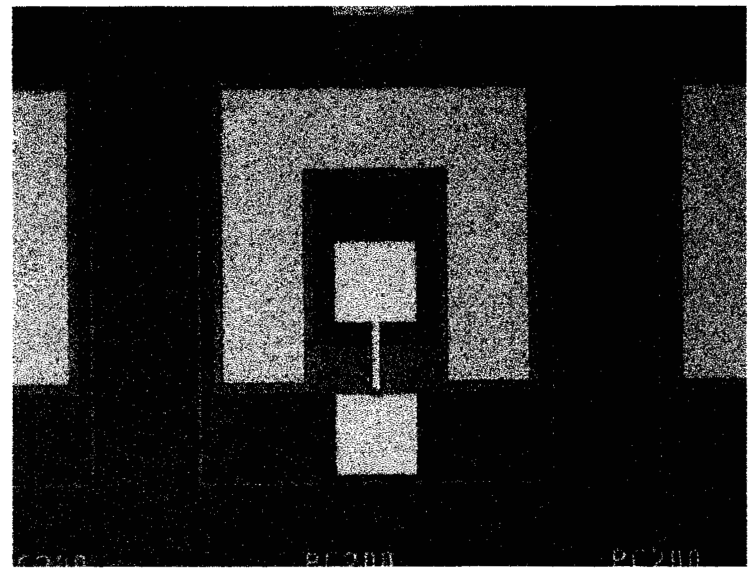
Task Lead: Doug Bell

Task Purpose/Objectives:

¥Develop a *room-temperature, radiation-tolerant* memory technology based on single-electron storage.

¥Decrease read/write time by orders of magnitude using a novel peaked-tunnel-barrier concept.

¥Increase capability for computing storage by increasing storage density and decreasing storage power.



Major Products:

¥Silicon nanocrystal floating-gate memory

¥Shape-engineered tunnel barrier for breakthrough read/write speed.

NASA Relevance:

¥**Space Science**: (autonomous spacecraft systems and robots)

¥**Earth Science**: (autonomous navigation / guidance; sensing and sensor webs)

¥**Human Exploration**: (autonomous robotic monitoring systems)

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Prepared by L. D. Bell 03 August 2000

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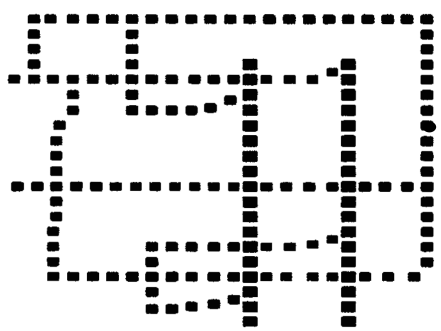
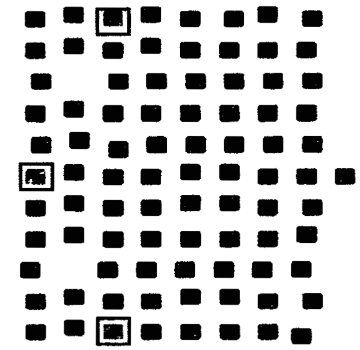
Quantum Dots Based Computing:

Quantum Dots Cellular Automata (QCA) Architectures and Applications

Task Lead: Amir Fijani



Novel QCA Circuits: A Bit-Serial Adder



Novel QCA Gates: Fault Tolerant Majority Gate

Objective:

¥ Develop new logic gates and circuits with emphasis on fault tolerance capabilities.

¥ Develop massively parallel computing architectures by exploiting inherent features of QCA.

Accomplishments:

¥ Alternative design of highly fault tolerant logic gates based on arrays of QCA.

¥ Massively parallel computing architectures for a set of signal/image processing applications.

NASA Relevance:

¥ Enable smaller and smarter spacecraft by providing drastic improvement over VLSI technology in terms of

- ¥ Integration density
- ¥ Mass, volume, and power consumption
- ¥ Radiationtolerance
- ¥ Enabling novel applications

External Collaborators:

¥ University of Notre Dame

¥ Oak Ridge National Laboratory

QCA: A totally new computing paradigm

Challenges: Architecture and Application Design, Fault Tolerance

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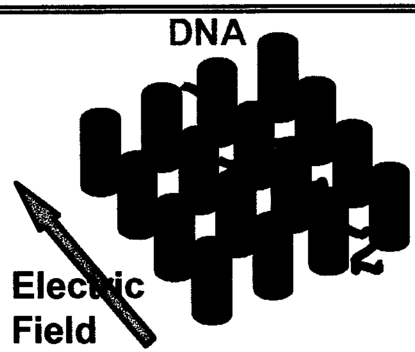
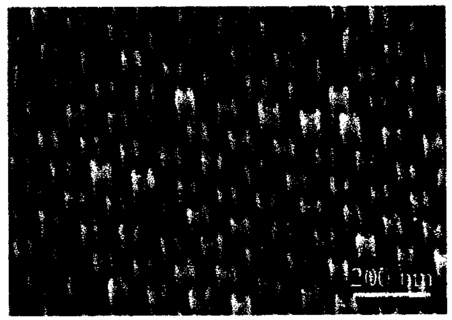
Bio-Inspired Nanotube Array Applications

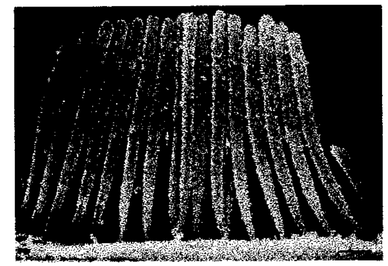
Task Lead: Brian Hunt



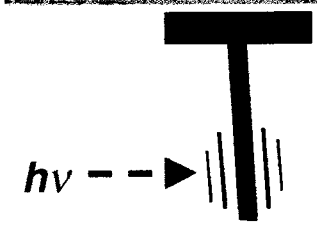
Nanotube-array electrophoresis system



Carbon nanotube array. Xu et al.



Biomimetic acoustic sensor



Mechanical signal processing

Motivation / Impact:

- Nanotubes combine useful properties and nanoscale dimensions
- NT-based electro-mechanical devices provide enabling technology for NASA missions: e.g., biomolecular probes, nanoexplorers

Objective:

Demonstrate prototype nanotube-based devices

- NT electrophoresis system
- Biomimetic acoustic sensor
- NT actuators
- NT high-Q resonators
- NT electronic components

NASA Applications:

- Search for life via acoustic and molecular signatures
- Nanoscale fabrication and characterization
- Revolutionary computing components
- Intense electron sources

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Motivation / Customers

- **NASA Relevance**:
  - Enable devices needed for NASA missions beyond existing industry roadmap:
    - 2-5μm lasers and detectors
    - High density, low power computation (logic and memory)
    - Life signature biosensors
- **Impact**:
  - Low cost development of revolutionary technology.
  - Narrow empirical/experimental search space
- **Customers / Missions**:
  - CISM
  - MDL
  - HPCC

Potential Benefits / Payoffs

NASA Relevance:

- 2-5mm Lasers and detectors
- High density, low power computation (logic and memory)
- Life signature biosensors

Impact:

- Narrow empirical/experimental search space
- Low cost development of revolutionary technology.

Quantum Dot Modeling - Development of Bottom-Up Nanoelectronic Modeling Tool

Delivery of a Simulation Tool

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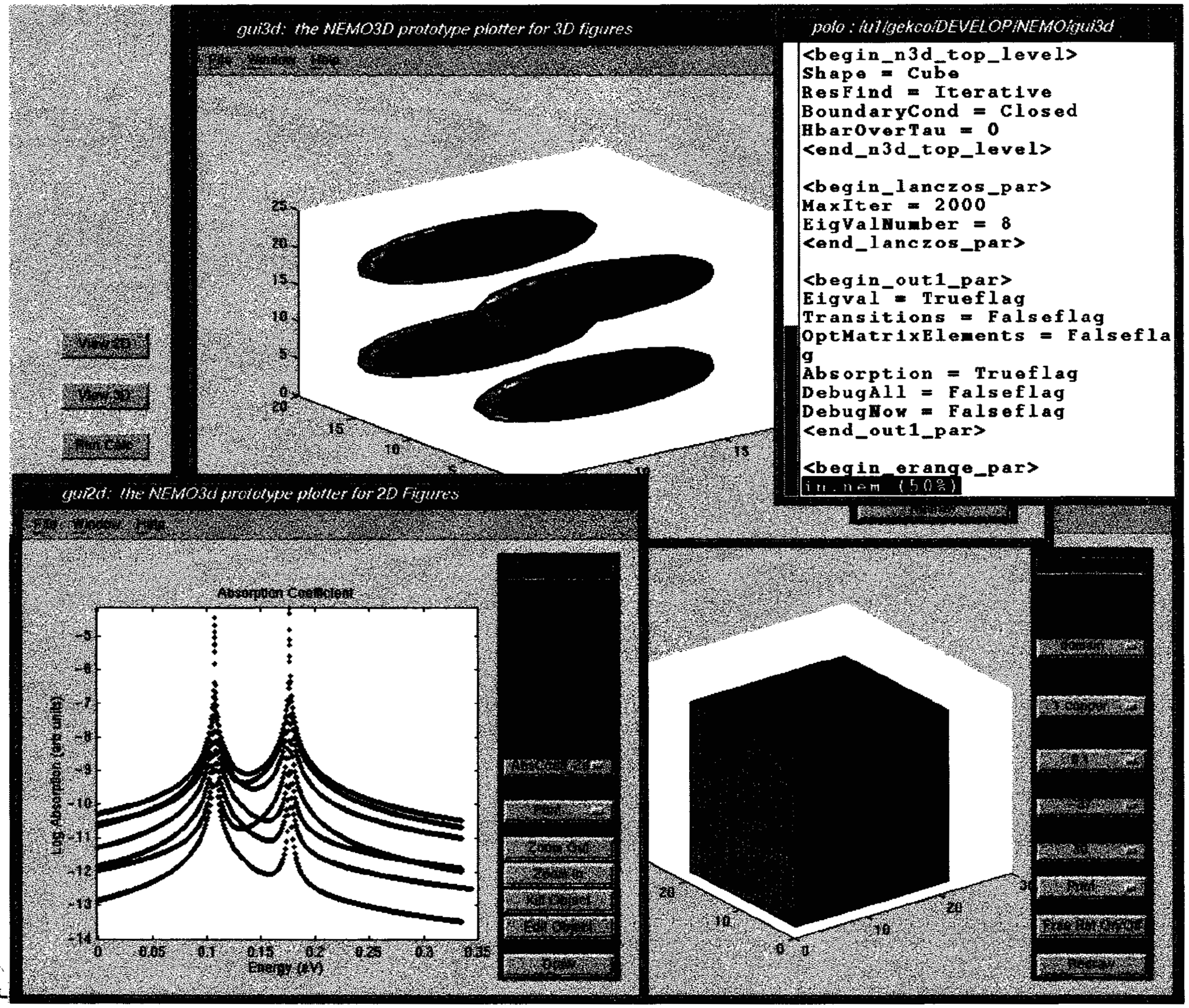

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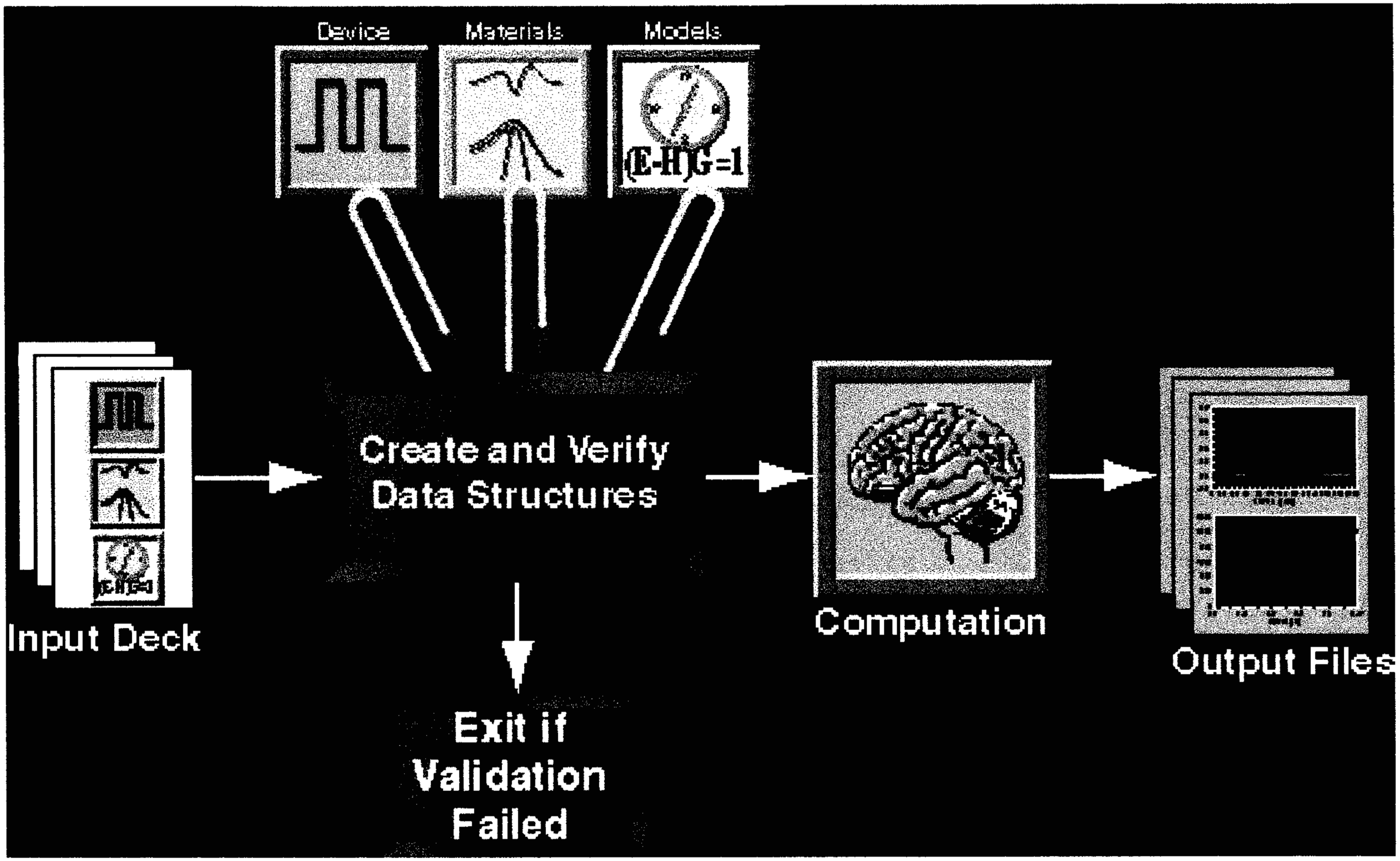
Batch Dataflow is Linear



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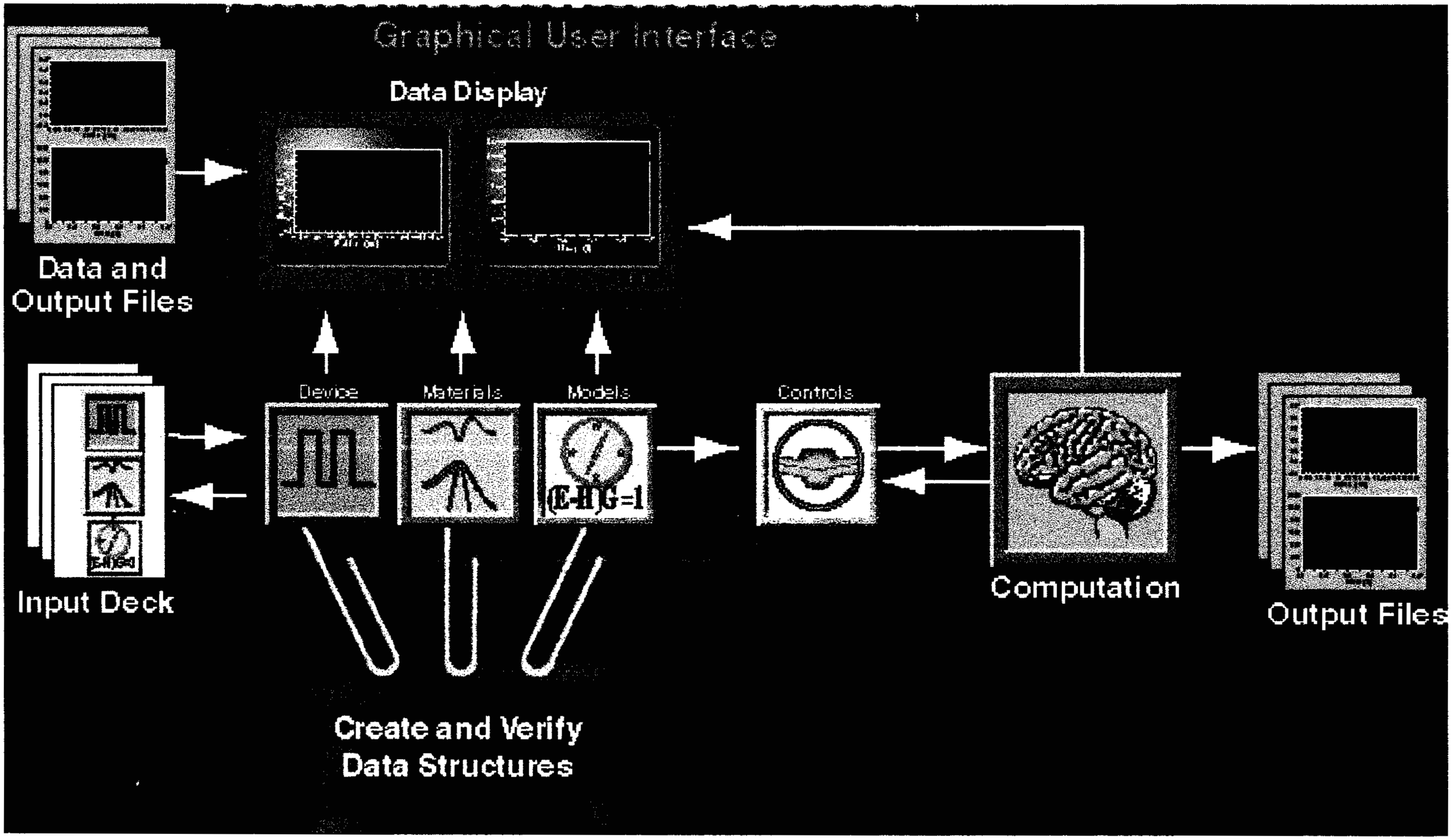
GUI Data Flow is Continuous



GUI interacts with different software blocks continuously

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Hierarchial Ordering of User Input

Semi-class. self-cons. pot. & single band current	Quantum self-cons. potential & single band current
	exchange & correlation?
	how to go from bias to bias?
Specify desired outputs	Specify desired outputs
Quantum region: "Where are wave-functions?"	Quantum region: "Where are wave-functions?"
Non-equilibrium region: "Where are the reservoirs?"	Non-equilibrium region: "Where are the reservoirs?"
	Quantum Charge region: "Where is the charge quantum mechanically calculated?"
Adaptive energy grid	Resonances-based energy grid

Ask user for input that is really needed.

-> User input determines the sequence of simulation parameter windows.

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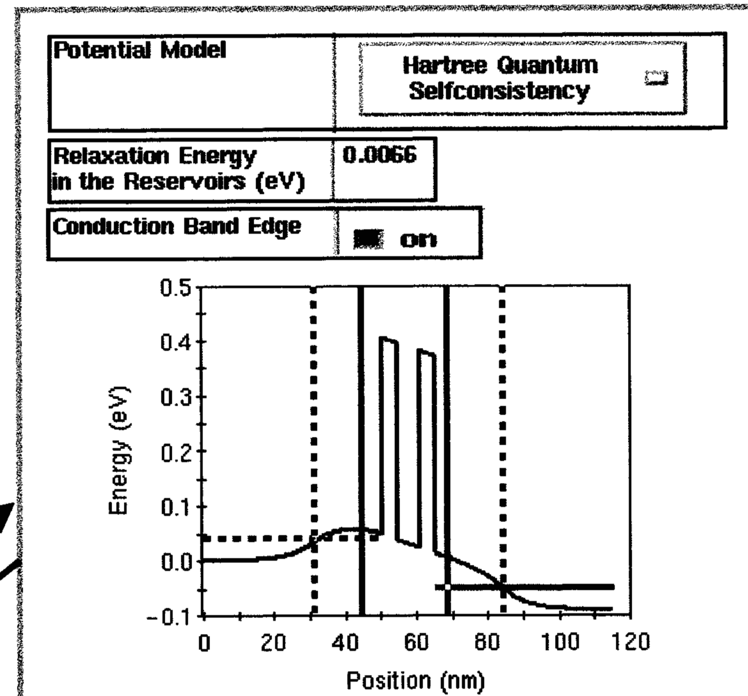
Generic Data Structure I/O

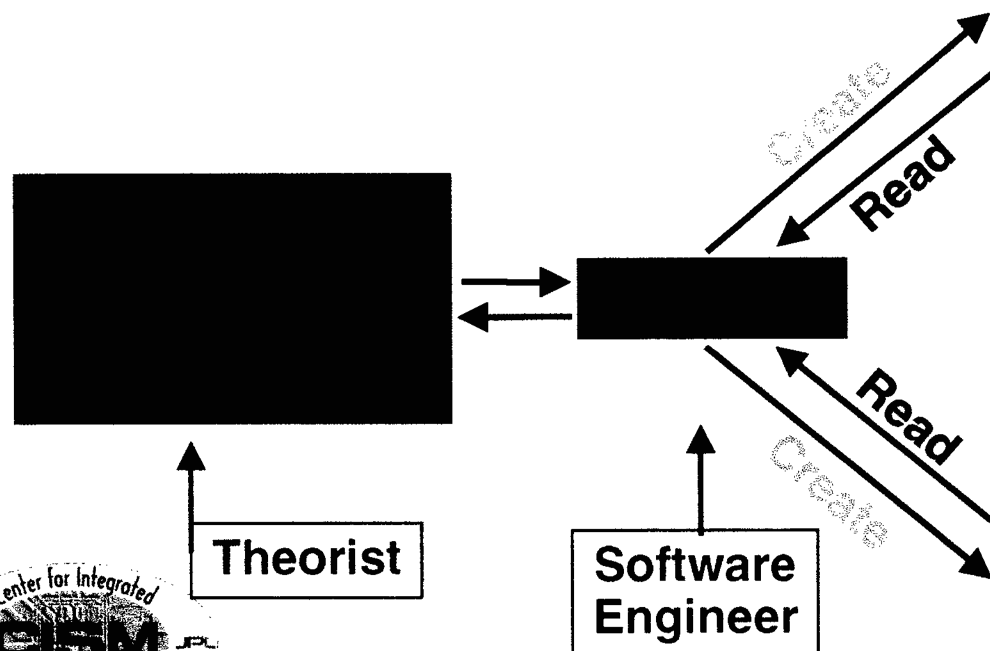
Dynamic GUI Design.

- data structure
- member descriptor

-> I/O for GUI or files



Graphical User Interface



File/Batch User Interface

```
potential=Hartree
hbarovertau=0.0066
Ec=FALSE
< start=45, end=69 >
```

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